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Time-Resolved Photoelectron Spectroscopy of Nitrobenzene and its Aldehydes

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Abstract

We report the first femtosecond time-resolved photoelectron spectroscopy study of 2-, 3- and 4-nitrobenzaldehyde (NBA) and nitrobenzene (NBE) in the gas phase upon excitation at 200 nm. In 3- and 4-NBA, the dynamics follow fast intersystem crossing within 1-2 picoseconds. In 2-NBA and NBE, the dynamics are faster (~ 0.5 ps). 2-NBA undergoes hydrogen transfer similar to solution phase dynamics. NBE either releases NO_2 in the excited state or converts internally back to the ground state. We discuss why these channels are suppressed in the other nitrobenzaldehydes.

Keywords: NO_2 release, intersystem crossing, internal conversion, excited state hydrogen transfer

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